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ORIGINAL ARTICLE

Simulating the impact between particles with applications in nanotechnology fields (identification of properties and manipulation)

M. H. Korayem · H. Khaksar · M. Taheri

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Abstract The aim of this research is to study and simulate the Andrews impact theory and its potential in identifying the properties of soft biological particles and in manipulating these particles at nano scale by means of the atomic force microscope (AFM). The reason for employing the Andrews theory in this research is that this theory is unique in considering the plastic state of soft biological nanoparticles. First, the required equations for the estimation of two basic parameters (i.e., indentation depth and contact radius) used in the identification of properties and manipulation of these particles were derived. Since none of the previous works has considered the velocity of biological nanoparticles, and since the impact of biological particles with AFM tip and with substrate has been ignored in these works, the impacts between AFM tip and DNA particle and between DNA particle and substrate were simulated in this paper. The findings showed that before applying a load to a particle by a cantilever, due to the impact of AFM tip with the particle, a relatively noticeable deformation was created. This deformation, which has been disregarded in previous works up to now, can play an important role in identifying the properties of nanoparticles, in manipulation and even in controlling the cantilever of the atomic force microscope. The existing experimental results were used to validate the findings of this research.

Keywords Andrews impact theory · Soft biological particles · AFM · DNA

Introduction

Today, with the proliferation of the science of robotics, this science is being developed in various fields. Of these areas are nanotechnology field and nanorobotics. AFM is one of the great achievements of this scientific advancement. The unique abilities of AFM in identifying the properties of unknown particles, producing accurate and flawless images of particles and their topography and in accurately manipulating various particles are some of the prominent features of this device. The indentation depth and the contact radius created in the events of contact and impact of AFM tip with nanoparticles constitute very important and basic parameters in the identification of particle properties and the manipulation-related issues including the estimation of critical force and time and even the control of AFM cantilever. Of the research done on this subject, Tranchida et al. used AFM and the contact theories to identify the properties of different particles. They explored the characteristics of various polymers using the computations related to indentation depth in the nano domain [1]. By developing a quantitative method, Sokolov et al. [2] identified the properties of biological nanoparticles based on AFM. They demonstrated how the elastic modulus of a cell body should be measured when the cellular brush is taken into consideration.

Li et al. employed AFM to compute and compare the elasticity moduli of two epithelial breast cancer cells. To determine the modulus of elasticity, this group compared the force–displacement diagram with that of the Hertz theory for spherical particles [3]. Wang et al. investigated and identified the viscoelastic properties of cancer cells using AFM [4].

M. H. Korayem (✉) · H. Khaksar · M. Taheri
Iran University of Science and Technology (IUST), Tehran, Iran
e-mail: hkorayem@iust.ac.ir

H. Khaksar
e-mail: Hesamkhaksar@mecheng.iust.ac.ir

M. Taheri
e-mail: Mtaheri@iust.ac.ir



Faria et al. used AFM to identify the elastic properties of prostate cancer cells. This group also benefitted from the Hertz contact theory for spherical nanoparticles [5]. Moeller employed AFM to investigate and obtain the properties and elasticity moduli of four different polymers by means of the indentation depth parameter in the nano domain [6]. Calabrie et al. also used AFM to study and identify the properties of various nanoparticles. This group presented a new method for nanoindentation based on the atomic force microscopy. In this research, they modeled AFM tip with a sharp point [7]. Regarding the subject of control, Korayem et al. carried out the analysis and control of an AFM microcantilever in the dynamic mode. In this paper, they modeled the interaction between tip and sample based on the Lennard-Jones potential. Based on this model, the phase image of the system was obtained according to the distance between tip and sample; and in the next section, the nonlinear behavior of cantilever was controlled. In this paper also, the studied particle had been considered as spherical [8]. Korayem and Omid studied the robust control of manipulation based on the atomic force microscopy. The model of Lennard-Jones potential was also used in this paper. To overcome the piezoelectric substrate motion control problems, control in the sliding mode was used [9].

Elasto-plastic impact theory of Andrews

Andrews [10] studied the contact between two spheres in the elasto-plastic mode as they impact each other with an initial velocity of V_0 . Based on Andrews theory, instead of the two spheres hitting each other, it is assumed that each sphere impacts a heavy rigid plate with a velocity half the initial velocity. Figure 1 shows the overall geometry of impact.

Figure 2 shows the problem algorithm. The process of contact can be divided into three steps.

In the first step, elastic compression occurs according to the classical theory of Hertz. This step starts from the moment

of contact and continues until the creation of a critical pressure (p'_0) at the surface of contact. Using Eq. 1 through (3), the initial parameters will be determined and then the required equations for all three regions will be presented.

$$\pi E_1^* = \frac{1 - \nu^2}{E}, E_2^* = 0 \quad (1)$$

$$K_1 = \frac{1}{m}, K_2 = \frac{4\sqrt{R}}{3\pi E^*} \quad (2)$$

$$R = \left(\frac{1}{R_1} + \frac{1}{R_2} \right)^{-1} \quad (3)$$

In the above equations, ν is the Poisson's ratio, E is the modulus of elasticity, m is the mass, R_1 is the radius of the investigated particle, and R_2 is the radius of AFM tip. Since, in the first step, contact has not entered the plastic zone yet, the force of the plastic region will be $F_p = 0$. Equations (4) through (6) yield the contact radius at the end of the first step, force vs. contact radius and force vs. indentation depth for the first step (elastic step), respectively.

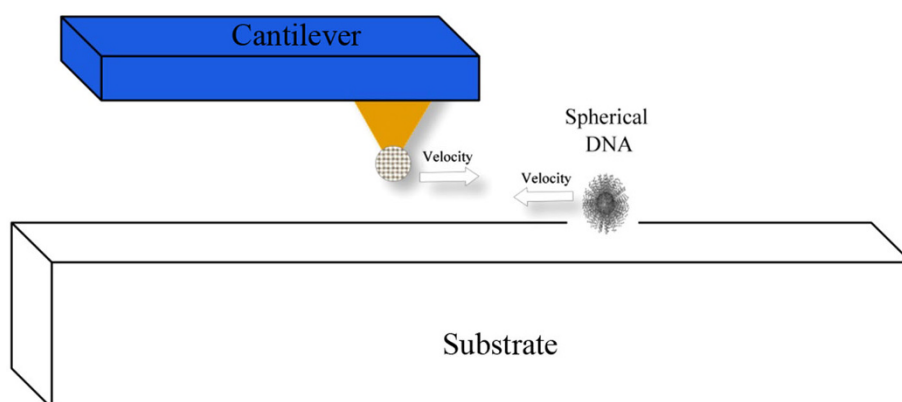
$$a_1 = \frac{\pi^2 R p'_0 E_1^*}{2} \quad (4)$$

$$F = F_p + F_E = \frac{4a^3}{3\pi E_1^*} \quad (5)$$

$$F = F_p + F_E = \frac{4}{3\pi E_1^*} (R\alpha)^{\frac{3}{2}} \quad (6)$$

In the second step of compression beginning with the end of the previous step, with the creation of a region confined by an elastic loop, the force of the plastic region increases with a constant pressure equal to the critical pressure; thus, the magnitude of F_p is no longer zero. Equations 7 and 8 express the plastic and elastic forces, respectively. Also, Eq. 9 indicates the relationship between force and indentation depth, and Eq. 10 represents the relationship between force and contact radius in the second step. At the end of this step, the radius is obtained from Eq. 11.

Fig. 1 Overall geometry of impact



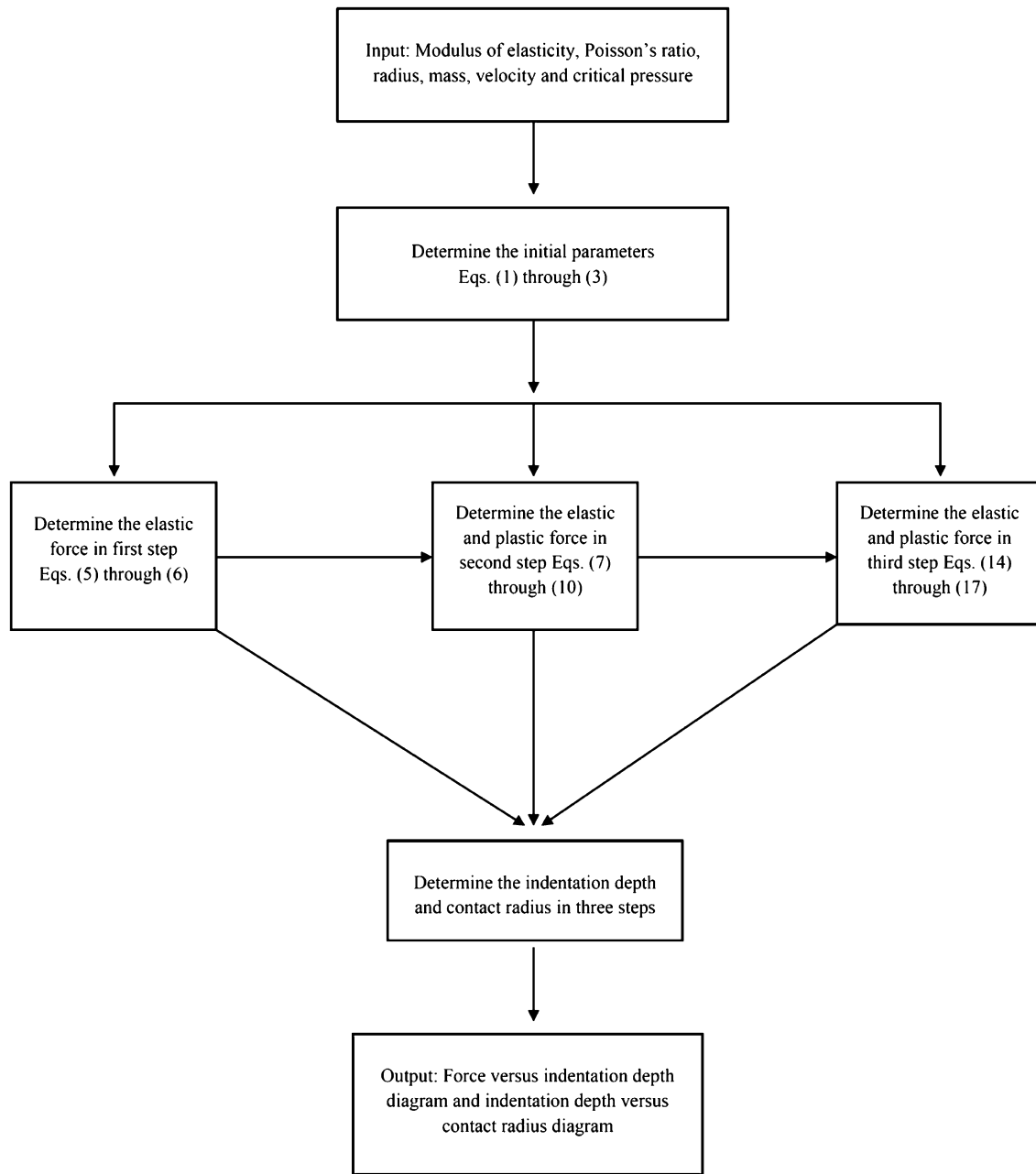


Fig. 2 Problem algorithm for Andrews theory

$$F_p = \pi(a^2 - R\alpha_1)p'_0 \quad (7)$$

$$F_E = \frac{2}{3}\pi R\alpha_1 p'_0 \quad (8)$$

$$F = F_p + F_E = \pi\left(R\alpha - \frac{1}{3}R\alpha_1\right)p'_0 \quad (9)$$

$$F = F_p + F_E = \pi\left(a^2 - \frac{1}{3}R\alpha_1\right)p'_0 \quad (10)$$

$$a_2 = \sqrt{R\left(\left(\frac{4}{9}\alpha_1^2 + \frac{\dot{\alpha}_1^2}{\eta^2}\right)^{\frac{1}{2}} + \frac{1}{3}\alpha_1\right)} \quad (11)$$

In the above equations, parameters η and $\dot{\alpha}_1$ have also been used. In fact, $\dot{\alpha}_1$ is the final velocity at the end of the first step. The values of these two parameters are determined by Eqs. 12 and 13.



$$\eta = \sqrt{\frac{\pi R}{m}} p'_0 \quad (12)$$

$$\dot{\alpha}_1 = \frac{v_0}{2} \sqrt{1 - \frac{16 K_1 k_2}{5 v_0^2} \alpha_1^{2.5}} \quad (13)$$

The third step is the reversal step. This stage of contact starts when the relative velocities of the two impacting objects become zero. In this step, the elastically confined plastic circle in the previous step reverses under the elastic pressure arising from the previous step. This reversal is such that the radius of the permanent deformation opening at the end of the reversal step becomes equal to the radius of the plastic radius in the second step. In this step, the equations associated with force are derived from Eqs. 14 and 15. Force vs. indentation depth and force vs. contact radius are represented by Eqs. 16 and 17 respectively. The contact radius at the end of the third step is determined from Eq. 18.

$$F_p = \frac{2r_1^{*2}}{R\pi E^*} \sqrt{a^2 - r_1^{*2}} \quad (14)$$

$$F_E = \frac{4(a^2 - r_1^{*2})^{\frac{3}{2}}}{3R\pi E^*} \quad (15)$$

$$F = F_p + F_E = \frac{2}{R\pi E^*} \left[\frac{2}{3} (R\alpha - r_1^{*2})^{\frac{3}{2}} - r_1^{*2} \sqrt{R\alpha - r_1^{*2}} \right] \quad (16)$$

$$F = F_p + F_E = \frac{2}{R\pi E^*} \left[\frac{2}{3} (a^2 - r_1^{*2})^{\frac{3}{2}} - r_1^{*2} \sqrt{a^2 - r_1^{*2}} \right] \quad (17)$$

$$\alpha_3 = \sqrt{R(\alpha_2 - \alpha_1)} \quad (18)$$

Parameter r_1^* has been used in the equations introduced for the third step. This parameter actually denotes the contact radius at the end of the third step. Equation 19 clearly defines this relationship.

$$r_1^* = \sqrt{R \left(\frac{4}{9} \alpha_1^2 + \frac{\dot{\alpha}_1^2}{\eta^2} \right) - \frac{2}{3} \alpha_1} = \sqrt{R(\alpha_2 - \alpha_1)} \quad (19)$$

Simulation of DNA

In 1953, Francis Crick and his colleague, Jim Watson, discovered the double helix structure of the DNA. By imaging the DNA and RNA molecules using the dynamic AFM, Keinberger et al. investigated the geometry and shape of the DNA molecule [11]. Komzolora et al. [12] studied the structure and the electrostatic properties of the DNA. Using the tapping mode of AFM, Yi et al. [13] identified the mechanical properties of the DNA. Studies have shown that the DNA molecule can be considered as a spherical pack at nano scale [14]. Therefore, to simulate this biological cell at contact moment, a spherical bundle of

Table 1 Properties of the biological DNA particle and Silicone [15]

Particles	Modulus of elasticity (G Pa)	Poisson's ratio
Silicone	169	0.27
DNA	0.1	0.35

DNA has been considered. Also, assuming DNA molecule to be cylindrical or circular capped cylinder, Korayem et al. [16] compared the contact mechanics of these two geometries with the results obtained from the spherical geometry, and concluded that the indentation depth created in the spherical geometry is greater than that produced in the other two types of geometries.

Simulating the theory of impact for use in the identification of properties and manipulation of nanoparticles

In this section, we simulate the impact of soft particles with AFM tip and with substrate. The significance of impact simulation lies in the fact that in all the simulation works performed so far, the velocity of biological particles has been overlooked; however, the living biological cells are moving and are not stationary. Manipulation is carried out in two ways. In the first case, AFM tip moves and the substrate remains fixed. In the second case, AFM tip is stationary and the substrate moves with a constant speed. The DNA molecule is the particle chosen for these simulations. Table 1 shows the properties of the biological DNA particle and the specifications of AFM tip and substrate (both made of Silicone). AFM tip radius and DNA particle radius were considered as 50 nm. In view of the given explanations, the simulation of impact is performed for two cases: first, when AFM tip is moving and second, when the substrate is moving with a constant speed. In both cases, the velocities of particles [17], AFM tip and substrate [18] were considered as 100 nm/s.

Figure 3 shows the simulation of the impact of DNA particle with the tip of AFM. Figure 3a, b shows the diagrams of force vs. indentation depth and indentation depth vs. contact radius, respectively. Figure 3a indicates that, due to the impact of the AFM tip on the particle, a very small force, but a noticeable indentation depth of about 0.6 nm, is produced on the upper surface of particle. The reason for the creation of this much indentation depth by such a slight force is the fact that the DNA particle is considered to have a plastic state. As Fig. 3b shows, with the increase of indentation depth, contact radius increases as well. In fact, for an indentation depth of about 0.6 nm, a contact radius of about 5.6 nm is created on the upper surface of particle due to impact before any force is applied by the cantilever.



Fig. 3 Simulation of the impact of DNA particle with the tip of AFM

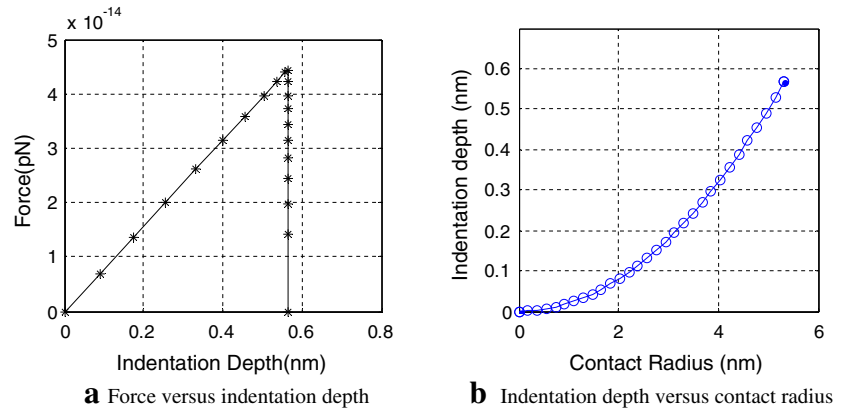


Fig. 4 Simulation of the impact of DNA particle with the substrate

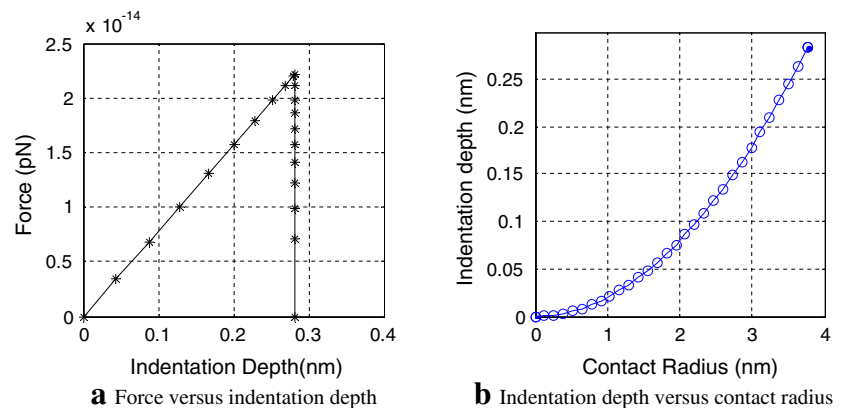


Figure 4 shows the simulation of the impact of DNA particle with the substrate. In view of Fig. 4a, we can see that the amount of indentation depth created in this case is about half the indentation depth produced by the impact of AFM tip with the particle. According to Fig. 4b, for this amount of indentation depth (about 0.3 nm), a contact radius of about 4 nm is produced on the bottom surface of particle. The interesting point is that, with the indentation depth becoming half as it was, the contact radius doesn't become zero. The reason that the forces in Figs. 3 and 4 approach zero is that in the elasto-plastic case of impact, the magnitude of force approaches zero in the third step. Of course, the amount of permanent deformation produced in the DNA particle due to impact is negligible. The reason is that the critical force of DNA is greater than the force created as a result of impact. Therefore, with this much force, the DNA particle doesn't exhibit a noticeable amount of plastic deformation.

To validate the Andrews theory, the EPH cell is simulated. By employing the atomic force bio-microscope, which is a hybrid type of AFM, Girot et al. [19] obtained the biological properties of the EPH cell. The EPH cell is considered as a soft material. The elasticity modulus and

the Poisson's ratio of this cell are about 28 kPa and 0.5, respectively.

To compute the indentation depth and to explore the contact mechanics of the EPH cell, Girot et al. assumed this cell to be spherical in shape with a radius of 5 μm . Their experimental results indicated that, by applying a load of up to 0.15 μN , this cell exhibits an elastic behavior. In this research, a silicon substrate was selected.

Considering the properties of the introduced cell and its small amount of deformation, the Hertz theory was applied for simulation purposes. Hertz theory describes the behavior of pseudo-elastic materials with small deformation. However, as observed in Fig. 5, at loads higher than 0.15 μN , the Hertz theory cannot properly justify the particle behavior. Nevertheless, by combining the Andrews impact theory with the Hertz contact theory, the results get closer to practical results, and a better answer is obtained.

Discussion and conclusion

There has been a lot of progress in the use of AFM in the field of nanotechnology, and this instrument is increasingly

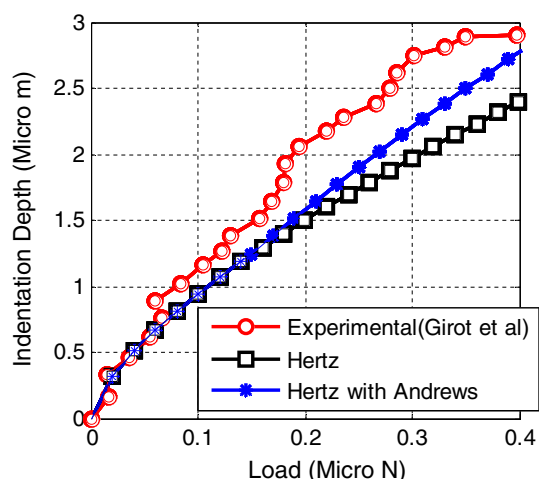


Fig. 5 Validate the Andrews theory

being exploited for imaging, properties identification and manipulation tasks. The most important notion regarding the manipulation-related simulations, identification of properties and the issues associated with the control of a manipulation process is the mechanics of contact. The mechanics of contact is actually initiated when a specific force is applied to the particle by AFM cantilever. But the important and appreciable point in the simulations that involve live biological cells is the impact of the considered particle with AFM tip and substrate before the load is applied by the cantilever. This is because the living biological cells are in motion; a fact that has been ignored in previous research works. Therefore, in this paper, we simulated the impact of soft particles.

The impact simulations in this paper were presented based on the elasto-plastic theory of Andrews. The Andrews theory is a three-step theory. In the first step, it considers the elastic state, in the second step, the elasto-plastic state, and in the third step, it considers the reversal and load carrying state. In this paper, the simulations were performed for two impact cases: the impact of AFM tip with DNA particle and the impact of DNA with substrate.

The results of contact radius simulations showed that, due to the impacts, contact radii of about 5.6 and 4.0 nm are obtained on the top and bottom surfaces of DNA, respectively. Also, the simulations of indentation depth indicated that the amount of indentation depth produced on the upper surface of the DNA particle is almost twice that produced on the lower surface. Therefore, in the simulations of contact, the impacts before the application of any load by AFM cantilever should be taken into consideration.

The existing experimental results were used to validate the simulation results. The findings indicated that the contact simulations that consider the impact of particles ahead of the application of load by AFM cantilever better match the existing empirical results in comparison with the

contact simulations that disregard the impact theory of Andrews. The final conclusion is that, for a better understanding of the manipulation process and a more thorough identification of the properties of biological particles, it is essential to consider the impacts that occur between particle, AFM tip and substrate.

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